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HAMILTONIAN FORM OF AN EXTENDED NONLINEAR SCHRÖDINGER EQUATION FOR MODELLING THE WAVE FIELD IN A SYSTEM WITH QUADRATIC AND CUBIC NONLINEARITIES

Yu. V. Sedletsky* and I.S. Gandzha

Abstract. We derive a Hamiltonian form of the fourth-order (extended) nonlinear Schrödinger equation (NLSE) in a nonlinear Klein–Gordon model with quadratic and cubic nonlinearities. This equation describes the propagation of the envelope of slowly modulated wave packets approximated by a superposition of the fundamental, second, and zeroth harmonics. Although extended NLSEs are not generally Hamiltonian PDEs, the equation derived here is a Hamiltonian PDE that preserves the Hamiltonian structure of the original nonlinear Klein–Gordon equation. This could be achieved by expressing the fundamental harmonic and its first derivative in symplectic form, with the second and zeroth harmonics calculated from the variational principle. We demonstrate that the non-Hamiltonian form of the extended NLSE under discussion can be retrieved by a simple transformation of variables.

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1. Introduction

Mathematical modelling of nonlinear waves in different physical systems has been a challenging task from both mathematical and computational points of view [1, 6, 28]. Here our focus is a simple physical system described by the nonlinear Klein–Gordon (nKG) equation with quadratic and cubic nonlinearities:

$$\phi_{tt} - c^2\phi_{xx} + \alpha_1\phi + \alpha_2\phi^2 + \alpha_3\phi^3 = 0. \tag{1.1}$$

The real function ϕ is a characteristic of the wave field and can have a mechanical, electromagnetic, quantum, nuclear, biophysical or other nature [35]. Equation (1.1) describes one-dimensional evolution of the wave field in time t, with x denoting a spatial coordinate and c being a velocity parameter that deals with the speed of interaction propagation (often the speed of light). The subscripts denote the partial derivatives. The real coefficients α_1, α_2 and α_3 are the parameters of the medium.

The nKG equation serves as a test bench in various fields of natural science to model nonlinear wave phenomena [21, 22, 32, 38]. For example, spatially localized oscillating nonlinear excitations of biological structures such as DNA chains can be described by the nKG equation with quadratic nonlinearity in the continuum limit [14]. Another direct application of the nKG equation is the quantum field theory where it is used to describe a

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Institute of Physics, National Academy of Sciences of Ukraine, Prosp. Nauky 46, Kyiv 03028, Ukraine.

* Corresponding author: sedlets@iop.kiev.ua

single relativistic scalar field and represents a relativistic field equation for scalar particles [40]. The potential $V = \frac{1}{2}\alpha_1\phi^2 + \frac{1}{3}\alpha_2\phi^3 + \frac{1}{4}\alpha_3\phi^4$ is a polynomial function of the field. When $\alpha_2 = 0$, equation (1.1) represents the celebrated ϕ^4 field model, which also has applications in elementary particle physics, statistical physics and condensed matter physics [24, 30]. When $\alpha_1 = 1$ and $\alpha_3 = -\frac{1}{6}$, the potential V represents the leading terms of the sine–Gordon model, which has multiple physical applications [13]. The term with α_2 (quadratic nonlinearity) describes additional ϕ^3 interactions. Quadratic nonlinearities are ubiquitous in nonlinear optics and other fields of nonlinear science [2, 8, 23]. The nKG model with quadratic and cubic nonlinearities was considered amongst others in references [17, 31, 39, 43].

When the wave packets exhibit slow modulations and have a narrow spectrum around the carrier frequency, they can be described by the nonlinear Schrödinger equation (NLSE). In the general context of weakly nonlinear dispersive waves, it was first discussed by Benney and Newell [5]. NLSE is formulated for the complex amplitude of the envelope of the wave field and takes into account the second-order dispersion and cubic nonlinearity [29, 41]. The slow-modulation approximation means the smallness of derivatives of the wave envelope, when oscillations noticeably change the amplitude for a time much longer than one oscillation. In this case, a significant change in the envelope occurs in time intervals of at least a dozen oscillations. For optical pulses this approximation is valid for pulse durations longer than a few tens of femtoseconds, depending on wavelength [26]. Modelling of ultrashort pulses (picosecond and femtosecond) or high-amplitude and steep waves (such as rogue waves) showed the insufficiency of the standard cubic NLSE to describe high-order dispersion and nonlinear effects [42]. High-order (extended) NLSEs need to be derived and used for this purpose.

The motive behind this paper is to derive an extended fourth-order NLSE

$$i\big(\psi_t + \omega_k\psi_x\big) + \tfrac{1}{2}\,\omega_{kk}\psi_{xx} + Q^{(3)}|\psi|^2\psi + i\big(-\tfrac{1}{6}\,\omega_{kkk}\psi_{xxx} + Q^{(4)}|\psi|^2\psi_x\big) = 0 \tag{1.2}$$

for the complex amplitude ψ of the envelope of some function (which will be defined further) of the wave field ϕ governed by the nKG equation (1.1). Here ω_k, ω_{kk} and ω_{kkk} are the first, second and third derivatives of the wave frequency ω with respect to the wave number k calculated at the point $k = k_0$, where k_0 is the carrier wave number. The coefficients $Q^{(3)}$ and $Q^{(4)}$ are real functions of the parameters of the original nKG equation. The standard cubic NLSE is given by the first three terms of equation (1.2) (the derivation of cubic NLSE can be found amongst others in reference [41] for the case $\alpha_2 = 0$). The last term in the brackets is a fourth-order extension of the cubic NLSE that takes into consideration the third-order dispersion and the nonlinear dispersion effects described by the first-order derivative $|\psi|^2\psi_x$ of the cubic nonlinear term. Equation (1.2) is missing another first-order derivative of the cubic nonlinear term, namely $\psi^2\overline{\psi}_x$ (the bar over ψ designates the complex conjugate). This makes it a Hamiltonian PDE, since the $\psi^2\overline{\psi}_x$ term has a non-Hamiltonian origin [36]. Such an extended Hamiltonian NLSE for the particular case of nKG equation with $\alpha_2 = 0$ was derived by Craig, Guyenne and Sulem in reference [10]. Our task is to extend their work to the case of quadratic nonlinearity (nonzero α_2).

The Craig–Guyenne–Sulem Hamiltonian approach is based on the elegant procedure of introducing a symplectic (coupled) coordinate-momentum variable, whose envelope is described by the amplitude ψ in equation (1.2). This approach preserves the Hamiltonian (symplectic) structure of the original nKG equation (1.1). The idea of using such coupled Hamiltonian variables belongs to Zakharov [44], but the symplectic formulation proposed by Craig, Guyenne and Sulem does not require transition to the Fourier space. The use of symplectic coordinates has two advantages: mathematical and physical. The mathematical advantage is that in a pair of Hamilton's equations for the coupled variable and its complex conjugate the second equation is a complex conjugate of the first one, which is also true for the NLSE. The physical aspect is that the new variable takes into account both a slow variation in the wave envelope and a contribution of the envelope motion during one fast oscillation.

When dealing with only the cubic nonlinearity ($\alpha_2 = 0$), it is sufficient to use only the first harmonic in the slow modulation approximation of the nKG equation (1.1) to get the fourth-order NLSE (1.2), as was done in reference [10]. The quadratic nonlinearity results in the generation of the second and zeroth harmonics in the same order of slow modulation approximation. In this paper, we combine the Craig–Guyenne–Sulem Hamiltonian approach to deal with the first harmonic and the Lagrangian approach, which is based on the variational principle, to properly take into account the input of the second and zeroth harmonics in the case of nonzero quadratic nonlinearity. We demonstrate that the second and zeroth harmonics generated by the quadratic nonlinearity make an important contribution to the nonlinear cubic coefficient $Q^{(3)}$ and to the nonlinear derivative coefficient $Q^{(4)}$.

The last point addressed in this paper is the relationship between the extended NLSE in Hamiltonian form (1.2) and the non-Hamiltonian form of the same equation derived earlier by the method of multiple scales [35], the method of averaged Lagrangian [16] and two-parameter method [27]. Recently we have proved the equivalence of these forms for the nKG equation with cubic nonlinearity [36]. Here we do the same for the case of coupled quadratic and cubic nonlinearity. We demonstrate that the non-Hamiltonian form of fourth-order NLSE can be retrieved by a simple transformation of variables. Such a transformation of variables was previously used in another context (dealing with different forms of water-wave envelope amplitude) in references [33, 34].

Summarising, the main purpose of this work is to extend the Hamiltonian approach of Craig, Guyenne and Sulem [10] to derive a Hamiltonian form of the fourth-order NLSE for the case of nKG equation with coupled quadratic and cubic nonlinearity. The second goal is to show that the result of reference [36] on the equivalence of Hamiltonian and non-Hamiltonian forms of the fourth-order NLSE obtained for case of cubic nonlinearity also holds for the case of quadratic nonlinearity coupled to the cubic nonlinearity.

2. Hamiltonian framework

2.1. Slow modulation approximation

In the linear case ($\alpha_2 = \alpha_3 = 0$), a solution to equation (1.1) is given by the fundamental harmonic, namely

$$\phi = \varphi = \Phi \exp\big(i(kx - \omega t)\big) + \text{c.c.},$$

where Φ is the complex amplitude of the wave field envelope (which stays constant) and c.c. stands for the complex conjugate. A relationship between the wave frequency ω and wave number k is given by the linear dispersion relation

$$\omega(k) = \sqrt{c^2k^2 + \alpha_1}. \tag{2.1}$$

In the weakly nonlinear approximation, the amplitude of the wave envelope is supposed to change slowly both in time and space, which leads to the slow modulation of the carrier (linear) wave. Such a slow modulation can be described in terms of the "slow" time $\tau = \varepsilon t$ and associated "long" coordinate $\chi = \varepsilon x$, where ε is a formal small parameter describing the slowness of wave modulations. Then the first harmonic of the wave field can approximately be written as

$$\varphi = \tfrac{1}{2}\,\varepsilon A(\chi, \tau) \exp(i\,\theta) + \text{c.c.}, \quad \theta = k_0 x_0 - \omega_0 t_0, \tag{2.2}$$

where $\varepsilon A \equiv 2\Phi$ is the complex amplitude of the first harmonic of the wave envelope, θ is the wave phase, k_0 is the carrier wave number, and $\omega_0 = \omega(k_0)$ is the carrier frequency. Note that here we associated the smallness of the wave amplitude with the same small parameter ε. It might not be always the best approach, as discussed in reference [27], but here for the sake of simplicity we assume that the slowness of wave modulation and the smallness of the wave field amplitude can be described by the same small formal parameter.

The slow modulation approximation assumes the amplitude A to be a function of "slow" time τ and "long" coordinate χ. At the same time, the wave phase is assumed to be a function of "fast" time $t_0 \equiv t$ and "short" coordinate $x_0 \equiv x$, so that it might be discarded by averaging on the slow time scale.

The relationship between different time and coordinate scales is given by the following perturbation expansions of differential operators:

$$\partial_t = \partial_{t_0} + \varepsilon\partial_\tau, \quad \partial_x = \partial_{x_0} + \varepsilon\partial_\chi. \tag{2.3}$$

To take into account the input of the quadratic nonlinearity, we model the wave field ϕ by a superposition of the fundamental, zeroth and second harmonics:

$$\phi = \varphi + \phi_0 + \phi_2. \tag{2.4}$$

In the slow modulation approximation, the zeroth and second harmonics are expressed in the same way as the fundamental harmonic:

$$\phi_0 = \varepsilon^2 A_0(\chi, \tau), \quad \phi_2 = \tfrac{1}{2}\,\varepsilon^2 A_2(\chi, \tau)\exp(2i\,\theta) + \text{c.c.} \tag{2.5}$$

They have the next order of smallness as compared to the fundamental harmonic because they are generated by the quadratic nonlinear term, while the fundamental harmonic is generated by the linear term in the nKG equation (1.1). Higher harmonics make no contribution to the fourth-order NLSE (1.2), which is our focus here, and we ignore them in ansatz (2.4).

2.2. Hamiltonian density in the nKG equation

The Hamiltonian density associated to the nKG equation (1.1) is

$$H = \tfrac{1}{2}\phi_t^2 + \tfrac{1}{2}c^2\phi_x^2 + \tfrac{1}{2}\alpha_1\phi^2 + \tfrac{1}{3}\alpha_2\phi^3 + \tfrac{1}{4}\alpha_3\phi^4. \tag{2.6}$$

Following the notation of reference [45], we split the Hamiltonian density into two parts,

$$H = H_2 + H_{\text{int}}. \tag{2.7}$$

The first part,

$$H_2 = \tfrac{1}{2}\big(\varphi_t^2 + c^2\varphi_x^2 + \alpha_1\varphi^2\big), \tag{2.8}$$

contains only those terms with the first harmonic φ that generate the linear (harmonic) part of the nKG equation. It is quadratic with respect to the first harmonic. The second part,

$$H_{\text{int}} = \Delta K + U_{\text{int}}, \tag{2.9}$$

contains all other terms. They produce the nonlinear part of the nKG equation, including all the terms with the second and zeroth harmonics as well as the nonlinear terms with the first harmonic. This part of the Hamiltonian density describes the wave interaction between different harmonics. Here

$$\Delta K = \tfrac{1}{2}\left(\phi_t^2 - \varphi_t^2\right) \tag{2.10}$$

is the difference between the kinetic energy densities of the wave field and first harmonic,

$$U_{\text{int}} = \tfrac{1}{2}c^2\big(\phi_x^2 - \varphi_x^2\big) + \tfrac{1}{2}\alpha_1\left(\phi^2 - \varphi^2\right) + \tfrac{1}{3}\alpha_2\phi^3 + \tfrac{1}{4}\alpha_3\phi^4 \tag{2.11}$$

is the density of potential energy without its harmonic part.

2.3. Symplectic representation of the first harmonic and Hamilton's equation

The last two terms of the Hamiltonian density H_2 are those that produce the right-hand side of the linear dispersion relation (2.1) after the transition to the Fourier space. Craig, Guyenne and Sulem [10] used this observation to introduce a Fourier multiplier operator such that the wave number k in the dispersion relation is replaced with the differential operator $-i\partial_x$:

$$\widehat{\omega} = \omega(-i\partial_x) = \sqrt{c^2(|-i\partial_x|\boxdot)^2 + \alpha_1(\boxdot)^2}. \tag{2.12}$$

Its action on some target function, whose position is indicated by symbol $\boxdot$, yields a nonpolynomial function of target function itself and its derivative. Such operators are also referred to as pseudo-differential operators [25].

The operator $\widehat{\omega}$ can be used to rewrite the Hamiltonian density H_2 in the following form:

$$H_2 = \tfrac{1}{2}(\varphi_t^2 + (\widehat{\omega}\varphi)^2) = \tfrac{1}{2}\big(i\varphi_t + \widehat{\omega}\,\varphi\big)\big(-i\varphi_t + \widehat{\omega}\,\varphi\big) = \sqrt{\widehat{\omega}}z\,\sqrt{\widehat{\omega}}\overline{z}. \tag{2.13}$$

Here the new variable

$$z = \frac{1}{\sqrt{2}}\Big(\sqrt{\widehat{\omega}}\,\varphi + i\frac{1}{\sqrt{\widehat{\omega}}}\,\varphi_t\Big) \tag{2.14}$$

is a complex symplectic coordinate that represents a coupling of the first harmonic φ and its derivative φ_t [10]. The inverse relationship between the functions $\{\varphi, \varphi_t\}$ and z is given by

$$\varphi = \frac{1}{\sqrt{2\widehat{\omega}}}\,(z + \overline{z})\,, \quad \varphi_t = \frac{\sqrt{\widehat{\omega}}}{\sqrt{2}i}\,(z - \overline{z})\,. \tag{2.15}$$

As noted in Introduction, our motivation to introduce a new variable comes from the goal of constructing an extended NLSE for the amplitude of the first harmonic and its complex conjugate as a pair of Hamilton's equations. The Hamilton equation for the complex symplectic coordinate z can be derived from Hamilton's principle (see Appendix A) in the following symmetric form:

$$iz_t = \frac{\delta\mathcal{H}}{\delta\overline{z}}, \tag{2.16}$$

where $\mathcal{H} = \int H dx$ is the Hamiltonian of the nKG equation and δ denotes the functional derivative. The second Hamilton equation for the function $\overline{z}$ is a complex conjugate of the first equation.

2.4. Operator expansions for the slow envelope

In the slow modulation approximation, the complex symplectic coordinate z can be represented in terms of its slow envelope and fast phase in the same way as we did it for the first harmonic φ:

$$z = \varepsilon u(\chi, \tau)\exp(i\theta). \tag{2.17}$$

Here εu is the complex amplitude of the envelope of function z. The amplitude u is a complex function of the slow time τ and long coordinate χ, while the phase θ is a function of fast time t_0 and short coordinate x_0.

Taking into account the perturbation expansion (2.3) of differential operator ∂_x, we have

$$-i\partial_x z = \varepsilon\exp(i\theta)\,(k_0 - i\varepsilon\partial_\chi)\,u. \tag{2.18}$$

The above formula allows us to formulate the following rule for the action of the Fourier multiplier operator $\widehat{\omega}$ on the function z:

$$\widehat{\omega}(-i\partial_x)\,z = \varepsilon\exp(i\theta)\,\widehat{\omega}(k_0 - i\varepsilon\partial_\chi)\,u(\chi). \tag{2.19}$$

The same rule is also valid for the operators $\sqrt{\widehat{\omega}}$ and $(\sqrt{\widehat{\omega}})^{-1}$. Note that such a rule for the action of Fourier multiplier operators on slowly modulated functions in a more general scope was rigorously proved in reference [12].

The operator $\widehat{\omega}$ in the right-hand side of relation (2.19) can be further expanded into power series in terms of small parameter ε describing the smallness of derivatives in the case of slow modulation of the wave envelope:

$$\widehat{\omega}(k_0 - i\varepsilon\partial_\chi) = \omega(k_0) + \sum_{n=1}^{\infty} \frac{\partial^n \omega(k)}{\partial k^n}\Big|_{k=k_0} (-i\varepsilon)^n \partial_{n\chi}.$$

The convergence and possibility of truncating this series at any finite order of n was proved in reference [12]. The same expansion can be written for the operator $\sqrt{\widehat{\omega}}$ in formula (2.13) for the Hamiltonian density H_2:

$$\sqrt{\widehat{\omega}\,(k_0 - i\varepsilon\partial_\chi)} = \sqrt{\omega_0}\left(1 + \sum_{n=1}^{3}(-i\varepsilon)^n l_n\,\partial_{n\chi}\right) + O(\varepsilon^4), \tag{2.20}$$

which we truncated at the order sufficient for the derivation of fourth-order NLSE (1.2). The expansion coefficients l_n are as follows:

$$\begin{aligned} l_1 &= \frac{\omega_0'}{2\omega_0}, & \omega_0' &= \omega_k(k_0) = \frac{c^2 k_0}{\omega_0},\\ l_2 &= \frac{\omega_0''}{4\omega_0} - \frac{\omega_0'^2}{8\omega_0^2}, & \omega_0'' &= \omega_{kk}(k_0) = \frac{c^2\alpha_1}{\omega_0^3},\\ l_3 &= \frac{\omega_0'''}{12\omega_0} - \frac{\omega_0'\omega_0''}{8\omega_0^2} + \frac{\omega_0'^3}{16{\omega_0}^3}, & \omega_0''' &= \omega_{kkk}(k_0) = -\frac{3c^4 k_0\alpha_1}{\omega_0^5}. \end{aligned} \tag{2.21}$$

With the expansion of the inverse operator,

$$\frac{1}{\sqrt{\widehat{\omega}\,(k_0 - i\varepsilon\partial_\chi)}} = \frac{1}{\sqrt{\omega_0}}\left(1 - i\varepsilon\rho_1\partial_\chi + O(\varepsilon^2)\right), \tag{2.22}$$

we can get an approximate relationship

$$A = \sqrt{\frac{2}{\omega_0}}\left(u - i\varepsilon\rho_1\, u_\chi + O(\varepsilon^2)\right) \tag{2.23}$$

between the amplitudes A and u, which follows directly from relation (2.15) for φ in terms of z. Here

$$\rho_1 = -\frac{\omega_0'}{2\omega_0} = -\frac{c^2 k_0}{2\omega_0^2}. \tag{2.24}$$

The inverse relationship,

$$u = \sqrt{\frac{\omega_0}{2}}\left(A - i\varepsilon\, l_1 A_\chi + O(\varepsilon^2)\right), \tag{2.25}$$

can be derived in a similar way from the relation $z + \overline{z} = \sqrt{2\widehat{\omega}}\,\varphi$. Note that a similar relationship between the amplitudes of canonical and non-canonical variables was also obtained in Fourier space in the framework of traditional Zakharov's Hamiltonian formalism in the theory of nonlinear surface water waves (see Eq. (B3a) from reference [19]). Is was also derived as a transformation between two different forms of water-wave envelope amplitude in references [33, 34].

3. Fourth-order NLSE as Hamilton's equation for the amplitude u

3.1. Hamilton's equation for the amplitude u

The evolution equation for the complex amplitude u of symplectic coordinate z is obtained from Hamilton's equation (2.16) by substituting relation (2.17) and expanding the differential operator ∂_t with the use of rule (2.3):

$$\varepsilon^2\omega_0 u + i\varepsilon^3 u_\tau = \frac{\delta\langle\mathcal{H}\rangle}{\delta\overline{u}}. \tag{3.1}$$

Here $\langle\cdot\rangle$ means averaging over the fast phase θ, which is a crucial step at this stage. The functional derivative in equation (3.1) is calculated as

$$\frac{\delta\langle\mathcal{H}\rangle}{\delta\overline{u}} = \frac{\partial\langle H\rangle}{\partial\,\overline{u}} - \frac{\partial}{\partial\tau}\frac{\partial\langle H\rangle}{\partial\,\overline{u}_\tau} - \frac{\partial}{\partial\chi}\frac{\partial\langle H\rangle}{\partial\,\overline{u}_\chi} + \frac{\partial^2}{\partial\chi^2}\frac{\partial\langle H\rangle}{\partial\,\overline{u}_{\chi\chi}} - \frac{\partial^3}{\partial\chi^3}\frac{\partial\langle H\rangle}{\partial\,\overline{u}_{\chi\chi\chi}} + \dots. \tag{3.2}$$

The averaged Hamiltonian density $\langle H\rangle$ in (3.2) can be expanded in a power series in terms of ε:

$$\langle H\rangle = \sum_{n=2}^{N}\varepsilon^n\langle H^{(n)}\rangle. \tag{3.3}$$

The same expansion can be written for the Hamiltonian $\mathcal{H}$. Summation starts with $n = 2$ because the minimum order of the Hamiltonian density is quadratic with respect to u and $\overline{u}$. To get a fourth-order NLSE from equation (3.1), it is sufficient to truncate the series in the fifth order ($N = 5$).

The Hamiltonian density H is a sum of two parts, H_2 and H_{int} (see formula (2.7)). The Hamiltonian density H_2 can be calculated by formula (2.13) with taking into account relation (2.17) and rule (2.19) applied for the operator $\sqrt{\widehat{\omega}}$, namely

$$H_2 = \varepsilon^2\Big(\sqrt{\widehat{\omega}\,(k_0 - i\varepsilon\partial_\chi)}\,u(\chi)\Big)\Big(\sqrt{\widehat{\omega}\,(k_0 + i\varepsilon\partial_\chi)}\,\overline{u}(\chi)\Big). \tag{3.4}$$

Taking into account operator expansion (2.20) and excluding the total derivatives with respect to χ (which disappear in the Hamiltonian $\mathcal{H}$ after integration with respect to χ), we get

$$H_2^{(2)} = \omega_0 u\overline{u},\ H_2^{(3)} = -\tfrac{1}{2}i\omega_0' u_\chi\overline{u} + \text{c.c.},\ H_2^{(4)} = -\tfrac{1}{4}\omega_0'' u_{\chi\chi}\overline{u} + \text{c.c.},\ H_2^{(5)} = \tfrac{1}{12}i\omega_0''' u_{\chi\chi\chi}\overline{u} + \text{c.c.} \tag{3.5}$$

Note that $\langle H_2\rangle = H_2$. The partial derivative of $\varepsilon^2 H_2^{(2)}$ with respect to $\overline{u}$ is identically equal to the term $\varepsilon^2\omega_0 u$ in the left-hand side of equation (3.1), and these two terms cancel out from the equation. Thus, equation (3.1) yields the following Hamilton equation for the amplitude u:

$$iu_\tau = \frac{\delta\langle\mathcal{H}^{(3)} + \varepsilon\mathcal{H}^{(4)} + \varepsilon^2\mathcal{H}^{(5)}\rangle}{\delta\overline{u}}, \tag{3.6}$$

where

$$\langle\mathcal{H}^{(3)}\rangle = \int H_2^{(3)} d\chi, \quad \langle\mathcal{H}^{(4)}\rangle = \int \big(H_2^{(4)} + \langle H_{\text{int}}^{(4)}\rangle\big) d\chi, \quad \langle\mathcal{H}^{(5)}\rangle = \int \big(H_2^{(5)} + \langle H_{\text{int}}^{(5)}\rangle\big) d\chi.$$

Due to the symplectic nature of variable z, the Hamilton equation for the function $\overline{u}$ is just a complex conjugate of the Hamilton equation for u.

The averaged Hamiltonian densities $\langle H_{\text{int}}^{(4)}\rangle$ and $\langle H_{\text{int}}^{(5)}\rangle$ are calculated by formula (2.9):

$$\langle H_{\text{int}}^{(4)}\rangle = \langle \Delta K^{(4)}\rangle + \langle U_{\text{int}}^{(4)}\rangle, \quad \langle H_{\text{int}}^{(5)}\rangle = \langle \Delta K^{(5)}\rangle + \langle U_{\text{int}}^{(5)}\rangle.$$

Expressions for the averaged densities of kinetic and potential energies are calculated by formulas (2.10) and (2.11). Omitting all the intermediate cumbersome but trivial algebraic transformations, we get

$$\langle \Delta K^{(4)}\rangle = \omega_0^2 A_2 \overline{A}_2, \quad \langle \Delta K^{(5)}\rangle = \tfrac{1}{2} i\omega_0 \overline{A}_2 (A_2)_\tau + \text{c.c.}, \tag{3.7}$$

$$\begin{aligned} \langle U_{\text{int}}^{(4)}\rangle &= \frac{3\alpha_3}{8\omega_0^2} u^2 \overline{u}^{\,2} + \frac{\alpha_2}{\omega_0} u\overline{u} A_0 + \Big(\frac{\alpha_2}{4\omega_0}\overline{u}^{\,2} A_2 + \text{c.c.}\Big) + \tfrac{1}{2}\alpha_1 A_0^2 + \big(\omega_0^2 - \tfrac{3}{4}\alpha_1\big) A_2 \overline{A}_2, \\ \langle U_{\text{int}}^{(5)}\rangle &= \frac{i\omega_0'}{2\omega_0^2}\Big(\frac{3\alpha_3}{4\omega_0} u\overline{u}^{\,2} u_\chi + \frac{\alpha_2}{2} u u_\chi \overline{A}_2 + \alpha_2 \overline{u} u_\chi A_0\Big) + \tfrac{1}{2} i c^2 k_0 A_2 (\overline{A}_2)_\chi + \text{c.c.} \end{aligned} \tag{3.8}$$

After calculating the functional derivative, equation (3.6) yields a fourth-order NLSE for the complex amplitude u. The last necessary step is to express the complex amplitudes A_0 and A_2 of the zeroth and second harmonics in terms of u. This can be done by means of variational approach.

3.2. Variational approach to calculating the amplitudes of zeroth and second harmonics

The complex amplitudes A_0 and A_2 of the zeroth and second harmonics can be found by the variational approach. A detailed record of the variational approach in application to the nKG equation can be found in reference [16]. It is based on minimising the action functional $S = \int \langle L\rangle d\chi$, where L is the Lagrangian density given by formula (A.1) from Appendix A. After expanding the averaged Lagrangian density in terms of ε,

$$\langle L\rangle = \sum_{n=2}^{N} \varepsilon^n \langle L^{(n)}\rangle, \tag{3.9}$$

variations need to be calculated separately in each order of n. In particular, expressions for A_0 and A_2 are obtained from the Lagrangian density of order $n = 4$, which is calculated as

$$\langle L^{(4)}\rangle = \langle \Delta K^{(4)}\rangle - \langle U_{\text{int}}^{(4)}\rangle.$$

The expressions for $\Delta K^{(4)}$ and $U_{\text{int}}^{(4)}$ are given by formulas (3.7) and (3.8). Calculating the functional derivatives of $S^{(4)} = \int \langle L^{(4)}\rangle d\chi$ with respect to A_0 and $\overline{A}_2$, we get expressions for A_0 and A_2 in terms of u:

$$A_0 = -\frac{\alpha_2}{\alpha_1\omega_0} u\overline{u}, \quad A_2 = \frac{\alpha_2}{3\alpha_1\omega_0} u^2. \tag{3.10}$$

Substituting these expressions in formulas (3.7) and (3.8), we eliminate the amplitudes A_0 and A_2 from the Hamiltonians $\mathcal{H}^{(4)}$ and $\mathcal{H}^{(5)}$ in Hamilton's equation (3.6). Now we can finally proceed to the derivation of fourth-order NLSE.

3.3. Fourth-order NLSE in Hamiltonian form

Hamilton's equation (3.6) contains Hamiltonians of different orders in parameter ε. To split these Hamiltonians apart and get a set of equations involving each of them separately, we have to introduce a multiscale expansion of the differential operator for slow time τ:

$$\partial_\tau = \partial_{t_1} + \varepsilon\partial_{t_2} + \varepsilon^2\partial_{t_3} + O(\varepsilon^3). \tag{3.11}$$

Here t_1, t_2 and t_3 are subtimescales, each of them being slower than the preceding one. This is a typical procedure in the multiple-scale approach [35]. Substituting such a multiscale expansion of time τ into equation (3.6), we get Hamilton's equations written for each of the time scales t_1, t_2 and t_3 separately.

Hamilton's equation with respect to time t_1 is

$$iu_{t_1} = \frac{\delta\langle\mathcal{H}^{(3)}\rangle}{\delta\overline{u}}.$$

This equation yields a linear equation describing the motion of the envelope with group velocity equal to ω_0':

$$iu_{t_1} + i\omega_0' u_\chi = 0. \tag{3.12}$$

Hamilton's equation with respect to time t_2 is

$$iu_{t_2} = \frac{\delta\langle\mathcal{H}^{(4)}\rangle}{\delta\overline{u}}.$$

It yields a cubic NLSE:

$$iu_{t_2} + \tfrac{1}{2}\omega_0'' u_{\chi\chi} + Q^{(3)}|u|^2u = 0, \tag{3.13}$$

where

$$Q^{(3)} = \frac{10\alpha_2^2 - 9\alpha_1\alpha_3}{12\alpha_1\omega_0^2} \tag{3.14}$$

is the cubic nonlinear coefficient.

Hamilton's equation with respect to time t_3 is

$$iu_{t_3} = \frac{\delta\langle\mathcal{H}^{(5)}\rangle}{\delta\overline{u}}.$$

It yields the evolution equation for the amplitude u in time t_3:

$$iu_{t_3} - i\tfrac{1}{6}\omega_0''' u_{\chi\chi\chi} + i\,Q^{(4)}|u|^2u_\chi = 0, \tag{3.15}$$

where

$$Q^{(4)} = \frac{2\omega_0'}{\omega_0}Q^{(3)} \tag{3.16}$$

is the cubic nonlinear derivative coefficient.

Finally, by summing up equation (3.12) multiplied by ε^2, equation (3.13) multiplied by ε^3 and equation (3.15) multiplied by ε^4 with taking into account expansion (3.11), we arrive at the following fourth-order NLSE for the complex amplitude u:

$$i\varepsilon^2\big(u_\tau + \omega_0' u_\chi\big) + \varepsilon^3\big(\tfrac{1}{2}\omega_0'' u_{\chi\chi} + Q^{(3)}|u|^2 u\big) + i\varepsilon^4\big(-\tfrac{1}{6}\omega_0''' u_{\chi\chi\chi} + Q^{(4)}|u|^2 u_\chi\big) = 0. \tag{3.17}$$

The second and zeroth harmonics generated by the quadratic nonlinearity make an important contribution to the nonlinear cubic coefficient $Q^{(3)}$ and nonlinear derivative coefficient $Q^{(4)}$, as can be seen from formulas (3.14) and (3.16). By making a simple transformation of variables

$$\psi = \varepsilon u, \quad \tau = \varepsilon t, \quad \chi = \varepsilon x,$$

we come to equation (1.2). This equation is a Hamiltonian PDE, inasmuch as it does not contain the non-Hamiltonian term with $\psi^2\overline{\psi}_x$. This is the final result of this paper.

Hamiltonian equation (3.17) can be transformed to the non-Hamiltonian form for the amplitude A by using relation (2.23) for A in terms of u. In this way, the Hamiltonian and non-Hamiltonian forms of the fourth-order NLSE can be shown to be equivalent in the case of coupled cubic and quadratic nonlinearities. More details are provided in Appendix B.

The wave field of the original nKG equation is expressed in terms of ψ as follows:

$$\phi(x,t) = \varphi + \phi_2 + \phi_0 = \sqrt{\frac{2}{\omega_0}}\Big(\mathrm{Re}\big(\psi\exp(i\theta)\big) - \frac{c^2 k_0}{2\omega_0^2}\,\mathrm{Im}\big(\psi_x \exp(i\theta)\big)\Big) + \frac{\alpha_2}{3\alpha_1\omega_0}\Big(\mathrm{Re}\big(\psi^2\exp(2i\theta)\big) - 3|\psi|^2\Big), \tag{3.18}$$

where $\theta = \omega_0 t - k_0 x$. The carrier wave number k_0 is a free parameter and the carrier frequency $\omega_0 = \omega(k_0)$ is determined from the linear dispersion relation (2.1).

4. Conclusions

This work is based on the Hamiltonian approach that was originally developed by Craig, Guyenne and Sulem in reference [10] to describe the modulation of weakly nonlinear dispersive waves. We extended this approach to the case of weakly nonmonochromatic waves involving several harmonics. To this end, we used an example of a simple physical system described by the nKG equation with quadratic and cubic nonlinearities. Besides the fundamental harmonic used in reference [10] to describe slowly modulated wave trains in such a system, we also took into account the second and zeroth harmonics. This allowed us to include the contribution of the quadratic nonlinearity to the fourth-order NLSE, which was derived in reference [10] only for the case cubic nonlinearity.

The fourth-order NLSE under discussion was proved to be a Hamiltonian PDE. It was derived from Hamilton's equation for a coupled variable that is a superposition of the first-harmonic amplitude and momentum. The second and zeroth harmonics were calculated by means of variational approach. Finally, we demonstrated that the non-Hamiltonian form of the same NLSE, which was derived by us earlier in references [16, 27, 35], could be retrieved by a simple transformation of variables. This proves the validity of the Hamiltonian approach used by us in this work in the case when the wave field is modelled by a superposition of several harmonics.

The Hamiltonian form of the fourth-order NLSE derived in this paper does not contain the non-Hamiltonian term that violates the conservation of energy. With the development of structure-preserving integrators, the conserved Hamiltonian (energy) makes such PDEs more attractive from the computational point of view [3, 7, 15, 20]. Further reading on the numerical integration of high-order NLSEs can be found amongst others in references [4, 11, 37].

Appendix A. Derivation of Hamilton's equation for z

The wave field $\phi(x,t)$ given by ansatz (2.4) is a function of the fundamental harmonic φ, zeroth harmonic ϕ_0 and second harmonic ϕ_2. We consider these three harmonics as independent variables. We also keep in mind the slow modulation approximation given by formulas (2.2) and (2.5).

The Lagrangian density for the nKG equation (1.1) can be written as

$$L = \tfrac{1}{2}\big(\varphi_t^2 - c^2\varphi_x^2 - \alpha_1\varphi^2\big) + \Delta K - U_{\text{int}}, \tag{A.1}$$

where U_{int} is given by formula (2.11). Substituting ansatz (2.4) into expression (2.10) for the difference of kinetic energy densities ΔK, we get

$$\Delta K = \tfrac{1}{2}\left(\phi_t^2 - \varphi_t^2\right) = \tfrac{1}{2}(\phi_0)_t^2 + \tfrac{1}{2}(\phi_2)_t^2 + (\phi_0)_t(\phi_2)_t + \varphi_t\big((\phi_0)_t + (\phi_2)_t\big). \tag{A.2}$$

The last two (cross) terms disappear after averaging over the fast phase θ. Therefore, they can be omitted in calculating the generalised momenta for the fields φ, ϕ_0 and ϕ_2:

$$p = \frac{\partial L}{\partial\varphi_t} = \varphi_t, \quad p_0 = \frac{\partial L}{\partial(\phi_0)_t} = (\phi_0)_t, \quad p_2 = \frac{\partial L}{\partial(\phi_2)_t} = (\phi_2)_t.$$

Hamilton's principle [9, 18] formulated in a phase space formed by the fields φ, ϕ_0, ϕ_2 and their momenta p, p_0, p_2 requires the functional

$$S[\varphi,\phi_0,\phi_2] = \int\big(p\,\varphi_t + p_0(\phi_0)_t + p_2(\phi_2)_t - H\big)\,dx \tag{A.3}$$

to keep a stationary value, so that $\delta S = 0$. Here H is the Hamiltonian density given by formula (2.6). Taking variations of S with respect φ and p, we come to a system of Hamilton's equations for these variables:

$$\varphi_t = \frac{\delta\mathcal{H}}{\delta p}, \quad p_t = -\frac{\delta\mathcal{H}}{\delta\varphi}, \tag{A.4}$$

where $\mathcal{H} = \int H dx$ is the Hamiltonian of the nKG equation.

Next we proceed to the equation for the complex symplectic coordinate z. By differentiating relation (2.14) with respect to t and taking into account equations (A.4), we get

$$iz_t = \frac{1}{\sqrt{2}}\left(\sqrt{\widehat{\omega}}\,i\frac{\delta\mathcal{H}}{\delta p} + \frac{1}{\sqrt{\widehat{\omega}}}\frac{\delta\mathcal{H}}{\delta\varphi}\right).$$

Calculating the functional derivatives

$$\frac{\delta\mathcal{H}}{\delta p} = \frac{i}{\sqrt{2\widehat{\omega}}}\left(\frac{\delta\mathcal{H}}{\delta z} - \frac{\delta\mathcal{H}}{\delta\overline{z}}\right), \quad \frac{\delta\mathcal{H}}{\delta\varphi} = \sqrt{\frac{\widehat{\omega}}{2}}\left(\frac{\delta\mathcal{H}}{\delta z} + \frac{\delta\mathcal{H}}{\delta\overline{z}}\right),$$

we come straightforward to the Hamilton equation (2.16) for the function z.

Appendix B. Fourth-order NLSE for the non-Hamiltonian amplitude A

Equation (3.17) for the amplitude u of the complex symplectic coordinate z can be rewritten in terms of the complex amplitude A of the first harmonic φ. To this end, we use relation (2.23) that expresses A in terms of u

and differentiate it with respect to τ. The terms with derivatives u_τ that appear in the right-hand side of the differentiated expression are calculated with the use of equation (3.17). After some algebraic transformations involving also relation (2.25) for u in terms of A, we come to the following fourth-order NLSE for the amplitude A:

$$i\varepsilon^2\big(A_\tau + \omega_0' A_\chi\big) + \varepsilon^3\big(\tfrac{1}{2}\omega_0'' A_{\chi\chi} + q^{(3)}|A|^2 A\big) + i\varepsilon^4\big(-\tfrac{1}{6}\omega_0''' A_{\chi\chi\chi} + q_1^{(4)}|A|^2 A_\chi + q_2^{(4)} A^2 \overline{A}_\chi\big) = 0. \tag{B.1}$$

The coefficients q_3 and $q_{1,2}^{(4)}$ are expressed in terms of the coefficients $Q^{(3)}$ and $Q^{(4)}$ present in the Hamiltonian NLSE (3.17) as follows:

$$q^{(3)} = \frac{\omega_0}{2} Q^{(3)}, \quad q_1^{(4)} = \frac{\omega_0}{2} Q^{(4)}, \quad q_2^{(4)} = \frac{1}{2} q_1^{(4)}.$$

After substituting relations (3.14) for $Q^{(3)}$ and (3.16) for $Q^{(4)}$, the above expressions for the coefficients $q^{(3)}$ and $q_{1,2}^{(4)}$ coincide with those we obtained earlier in deriving high-order non-Hamiltonian NLSEs for the amplitude A by the method of multiple scales [35], the method of averaged Lagrangian [16] and two-parameter method [27]. This proves the equivalence between the Hamiltonian and non-Hamiltonian forms of the fourth-order NLSE for the nKG equation with coupled quadratic and cubic nonlinearities. The non-Hamiltonian form of fourth-order NLSE (B.1) can be retrieved from the Hamiltonian form (3.17) by a simple transformation of variables.

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